Adjoint Computational Electrodynamics

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The adjoint method is used to inverse design linear and nonlinear photonic devices. The purpose of this handout is give the reader an introduction to the topic.

Motivation

In normal electromagnetic simulation, we are given a material distribution represented by $(\epsilon(x,y,z), \mu(x,y,z))$ and a current density source $\mathbf{J}(\mathbf{x},\mathbf{y},\mathbf{z})$. Maxwell's equations are then solved using one of the computational techniques (FD, FEM, MoM) for the excited electromagnetic field $(\mathbf{H},\mathbf{E})$. For linear, isotropic, non magnetic and stationary media [1] $\mathbf{B} = \mu_0\mathbf{H}$ and $\mathbf{D} = \epsilon\mathbf{E}$. Maxwell's equations take the form

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \tag{1a}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \epsilon \frac{\partial \mathbf{E}}{\partial t} \tag{1b}$$

[1] In general ϵ and μ may be nonlinear anisotropic tensors. We restricted ourselves to linear isotropic media for simplicity and most material are nearly the case.

We are asked to maximize the scaler quantity $G(\mathbf{E},\mathbf{H})$ by varying the dielectric structure $\epsilon(x,y,z)$. G is often a measure of device performance: for example, the power flowing in certain direction or mode conversion efficiency. This is an inverse design problem, we start by defining an objective G and ask for the best material distribution to achieve this objective.

The gradient quantity $\frac{dG}{d\epsilon}$ is useful to compute. It could be used as a measure of robustness and sensitivity to any structure deformations like fabrication imperfections. In inverse design, it is the major quantity needed as it points in the direction of steepest ascent, from which we have an informed decision of how to update the dielectric structure.

$$\epsilon \longleftarrow \epsilon + \alpha \frac{dG}{d\epsilon} \tag{2}$$

Where α is the step size in the gradient direction[2].

[2] Some algorithms attempt to optimize the step size so that the step maximally increases G

Assuming we have n number of design points, to calculate the sensitivity $\frac{dG}{d\epsilon}$ there are different approaches which vary in complexity and accuracy. One way is by using a finite difference approximation $\frac{dG}{d\epsilon} \approx \frac{\Delta G}{\Delta \epsilon}$. In this approach we need to carry n number of forward simulations. For a typical $100 \times 100 \times 100$ 3D finite difference grid, this means 1000000 simulations!. This approach also suffers from numerical discretization errors and the need to determine how small or

large is $\Delta\epsilon$. Automatic differentiation can be used to get the derivative exactly. However, there are are two modes in automatic differentiation. The automatic forward mode, like finite difference, needs n number of forward simulations. In the automatic adjoint or reverse mode, two simulations are only needed regardless of the number of the design points. So, the adjoint method is by far much better in accuracy than finite difference and computational cost than automatic forward differentiation.